# Generation IV Reactors
Neutron Thermalization
&
Neutronics-Materials Interface

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Nuclear Reactor Program

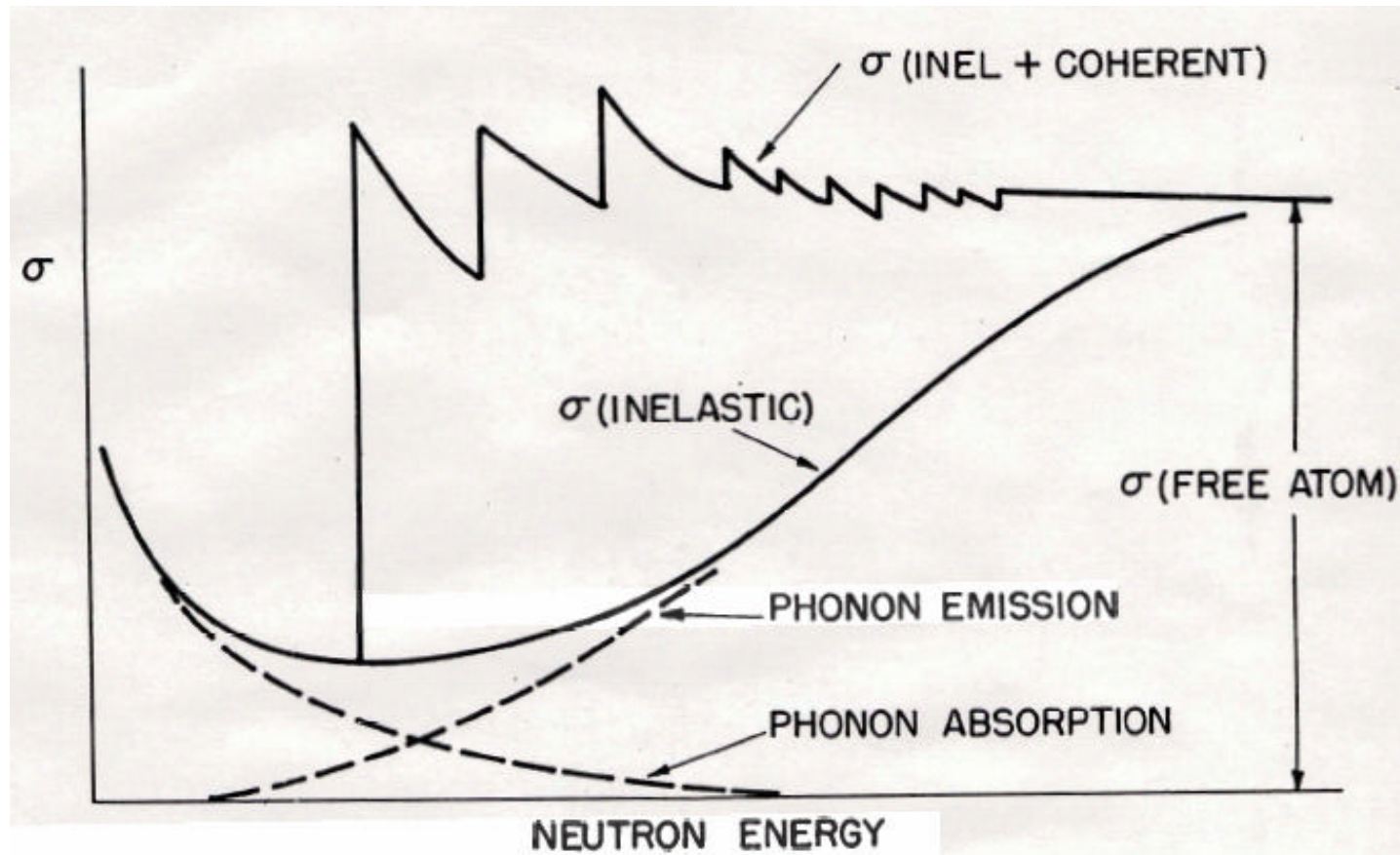## Nuclear Engineering

North Carolina State University

Generation IV Reactors

- Several concepts

- VHTR is a thermal, graphite moderated and reflected reactor
  - NGNP is a demonstration VHTR
    - Prismatic fuel
    - Pebble bed

- How well do we understand neutron thermalization in graphite?
  - NERI-2001 with ORNL

Neutronics
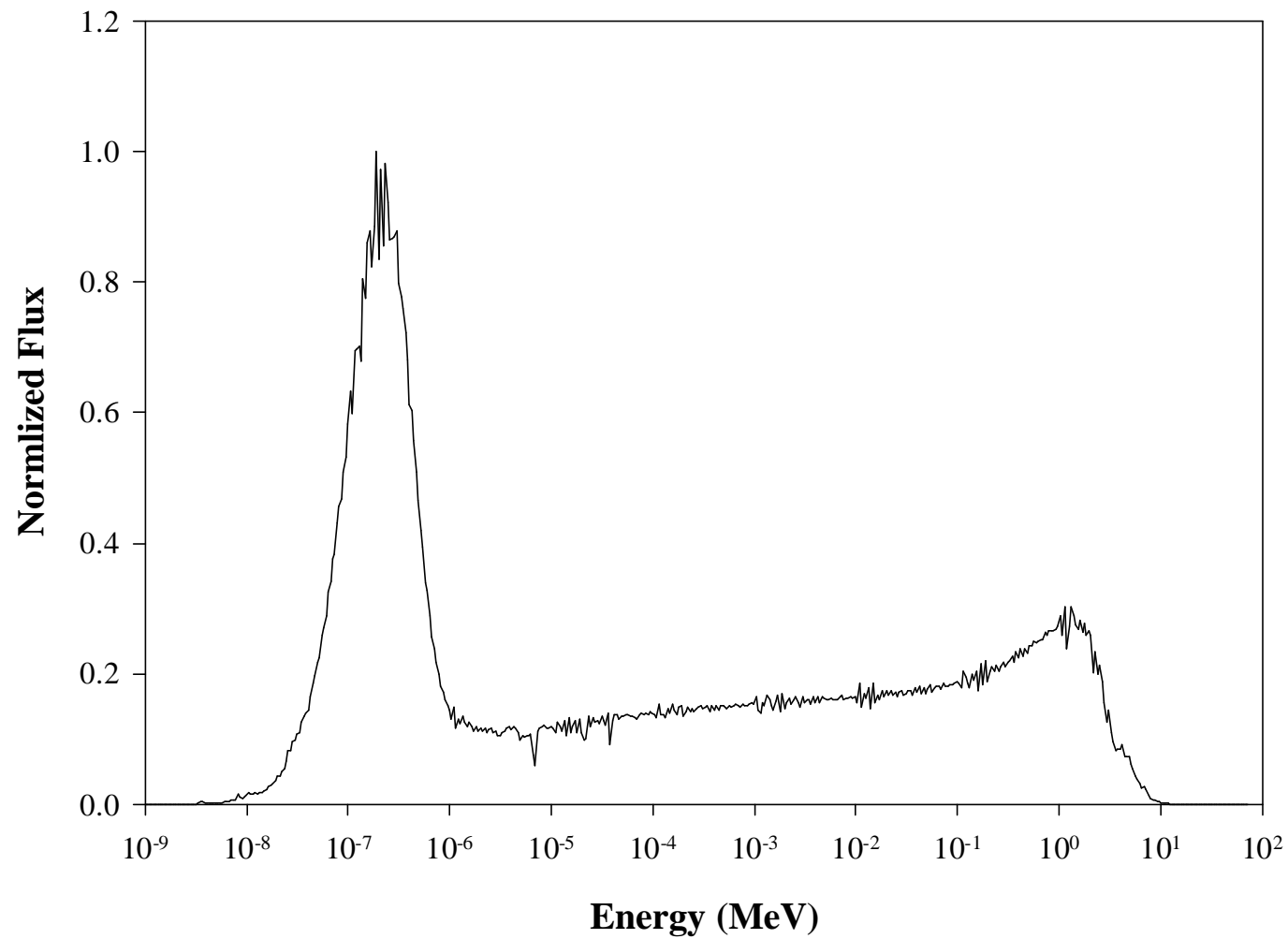
Thermal Neutron Scattering

$$\frac{d^2\sigma}{d\Omega dE}\bigg|_{inelastic} = \frac{\sigma}{2k_B T}\sqrt{\frac{E'}{E}}e^{-\frac{\beta}{2}}S(\alpha,\beta)$$

$$\beta = \frac{E - E'}{k_B T} \quad \text{Energy Transfer} \qquad \alpha = \frac{(E + E' - 2\sqrt{EE'}\cos\theta)}{k_B T} \quad \text{Momentum transfer}$$

The scattering law is the Fourier transform of a correlation function

$$S(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-i\beta t}e^{-\gamma(t)}dt$$

$$\gamma(t) = \frac{\alpha}{2}\int_{-\infty}^{\infty}\frac{\rho(\beta)}{\beta\sinh(\beta/2)}\left[1 - e^{-i\beta t}\right]e^{\beta/2}d\beta$$

$\rho(\beta)$ phonon (vibration) frequency distribution

Unirradiated Graphite

Perfect graphite consists of planes (sheets) of carbon atoms arranged in a hexagonal lattice. Covalent bonding exits between intraplaner atoms, while the interplaner bonding is of the weak Van der Waals type. The planes are stacked in an "abab" sequence.
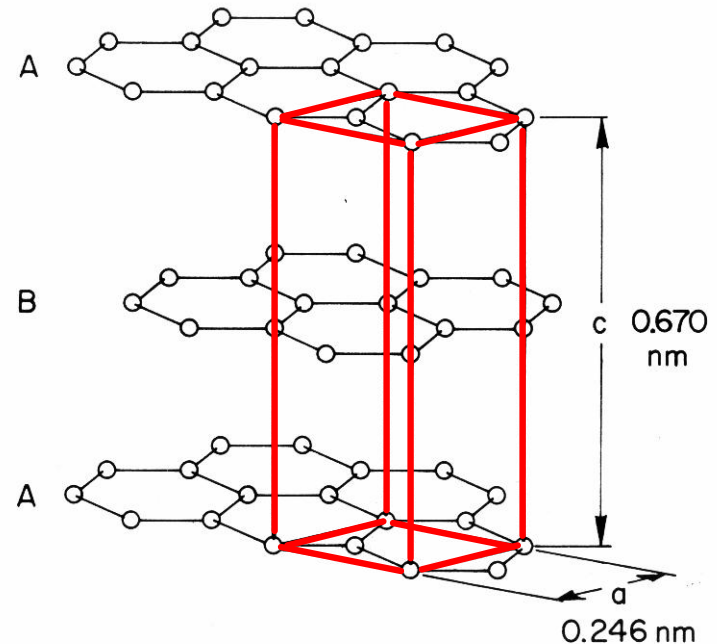
- ☐ Hexagonal Structure
- ☐ 4 atoms per unit cell
- ☐ a=b=6.7 Å
- ☐ c=2.46 Å

Graphite Benchmark
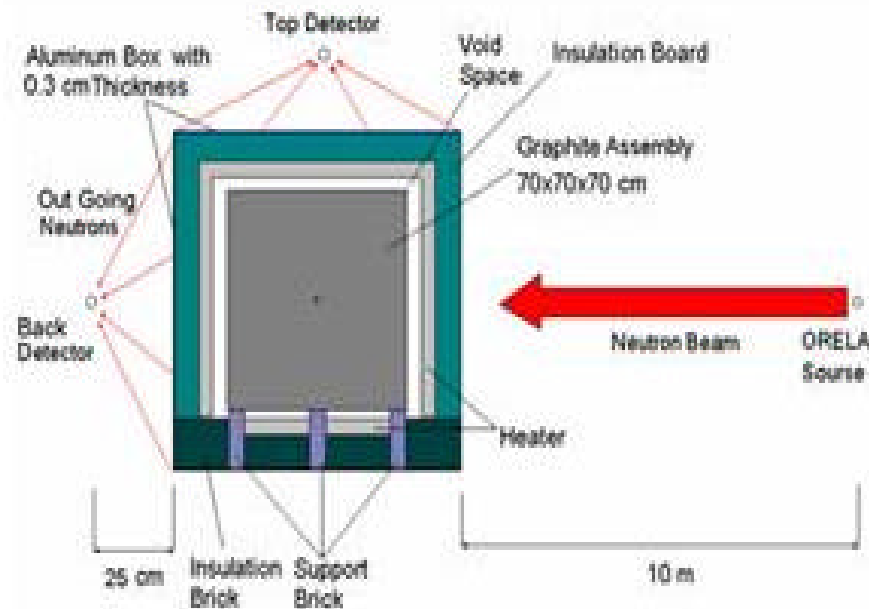
Moderator Microstructure Considerations

- ☐ The VHTR (prismatic or pebble bed) is designed as a gas cooled and graphite moderated reactor

- ☐ The graphite will be exposed to neutron irradiation, which inevitably will cause changes in the microstructure of graphite

- ☐ Changes in microstructure will be fluence dependent. Therefore, the graphite microstructure will change with time

- ☐ The thermal scattering cross section is microstructure dependent and can potentially change as a function of exposure (time)

Imperfect Graphite – Radiation Damage

- Upon irradiation, the graphite structure is disrupted through the formation of vacancies and interstitials.
- Due to their greater mobility, the interstitials diffuse and take position between the planes and coalesce to form chains of linear molecules (C_2, C_3, C_4, etc.).
- As the linear molecules become large, they are postulated to transform and form hexagonal covalently bonded clusters.
- This eventually leads to the formation of interstitial "c" planes between the hexagonal "abab" layers.
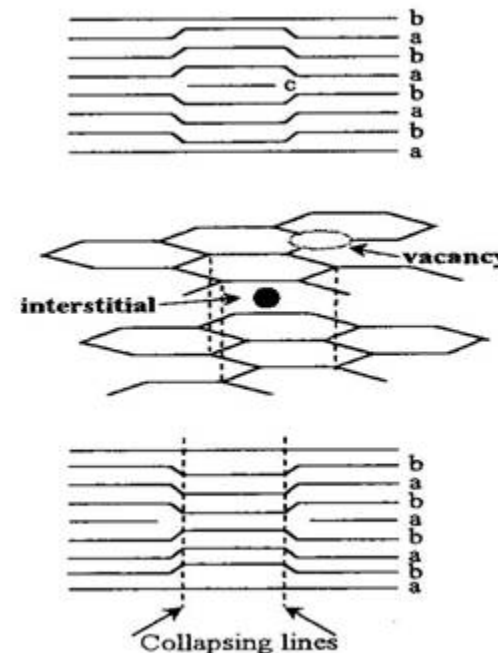
- Structure ????
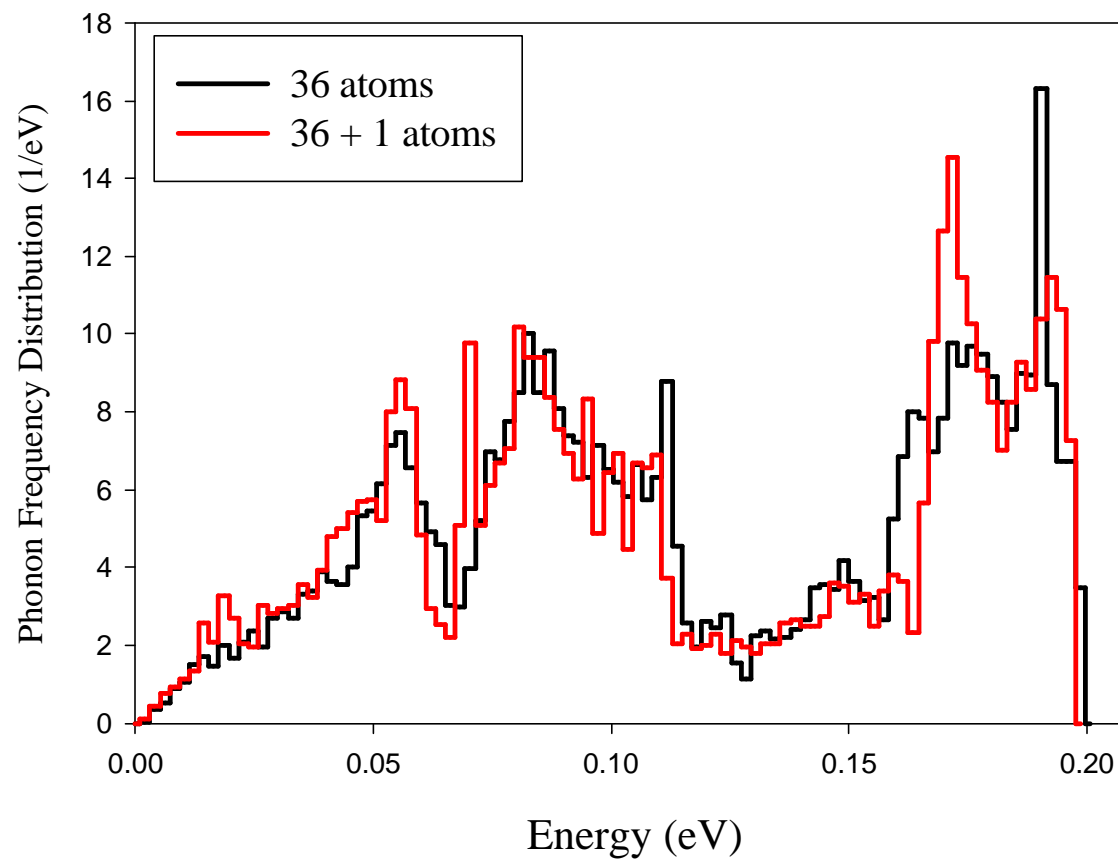- Basel plane contract
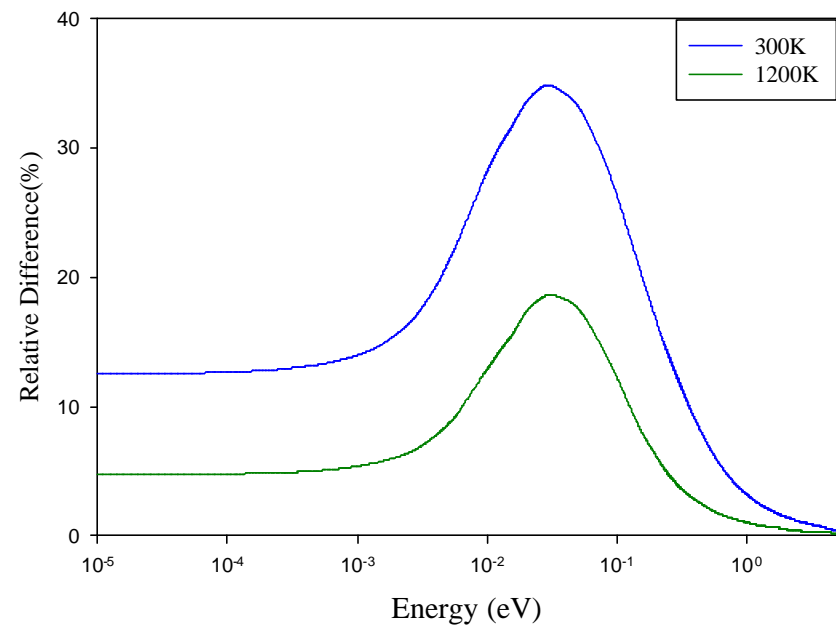- c expansion

Imperfect Graphite
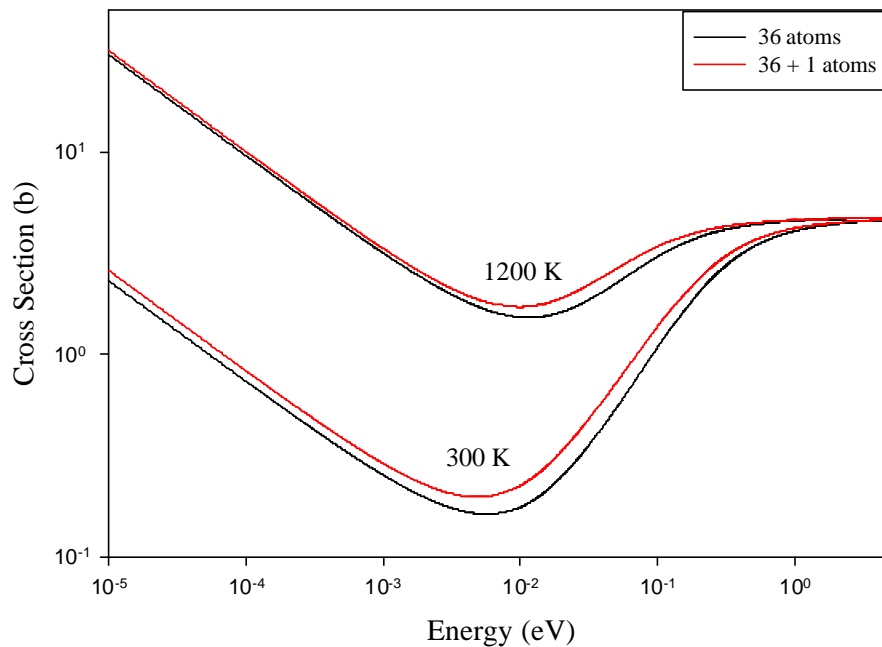# Single and Di-interstitials
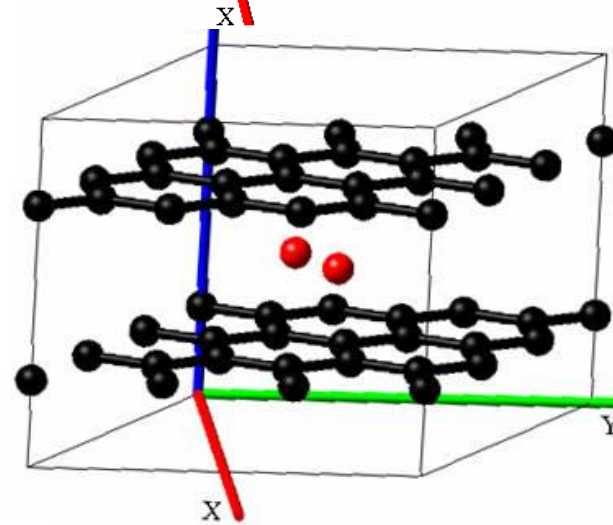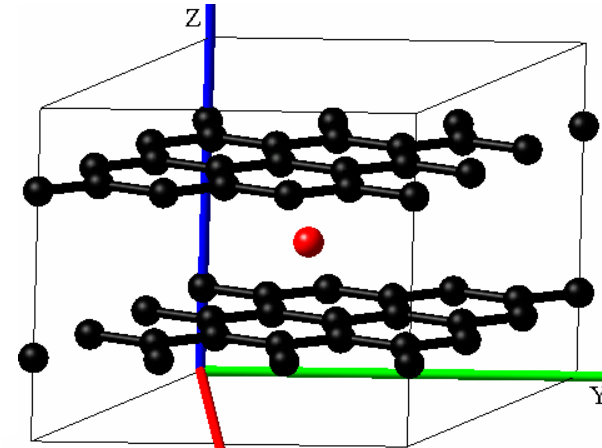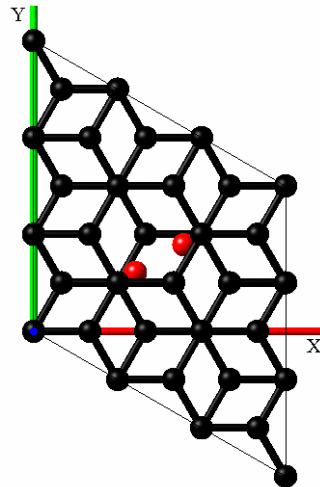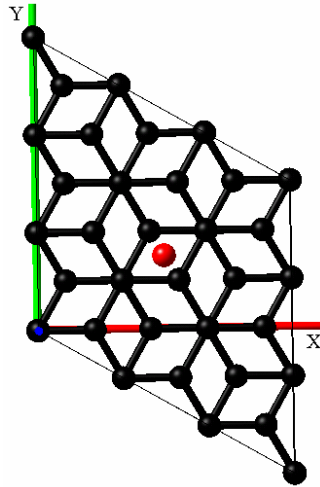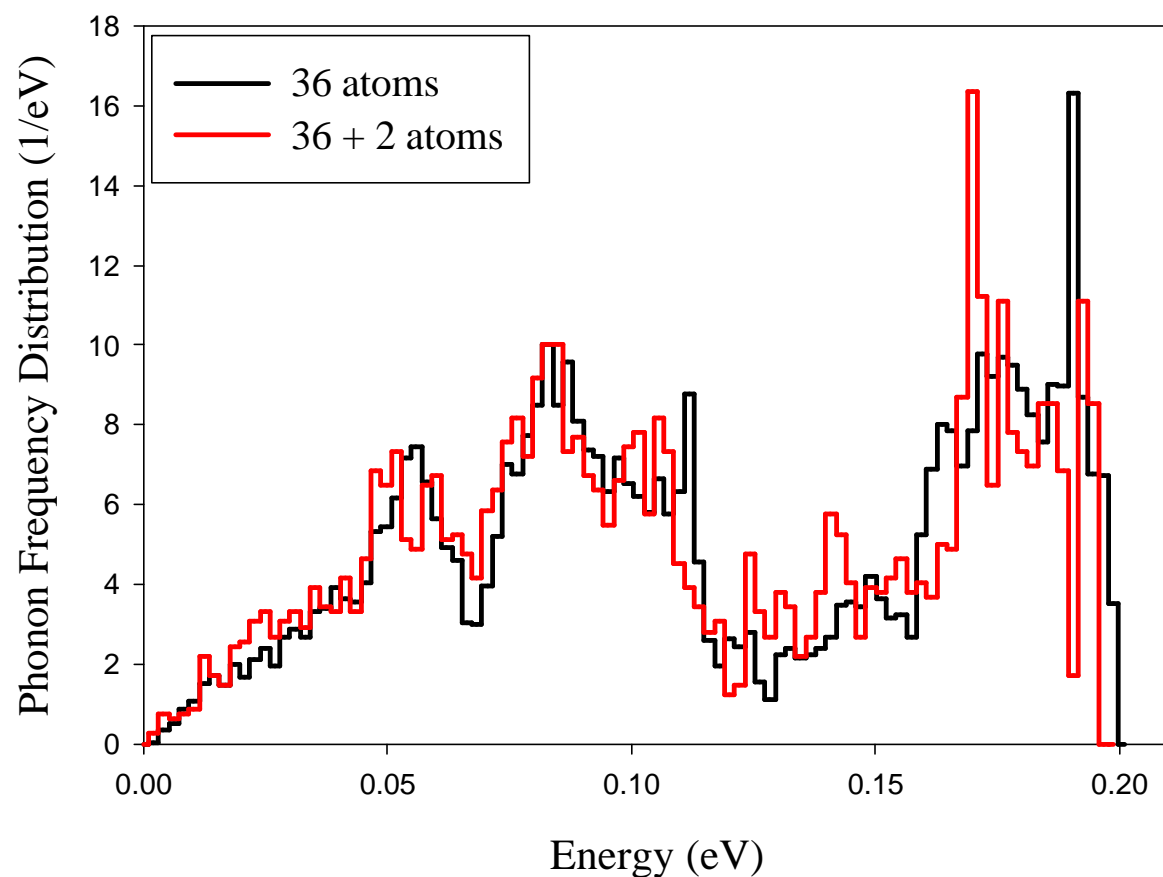
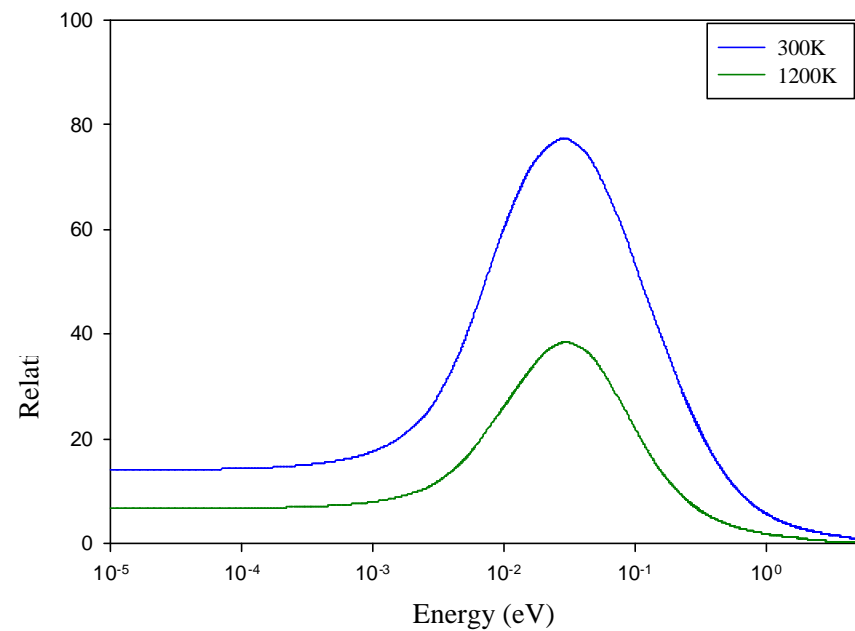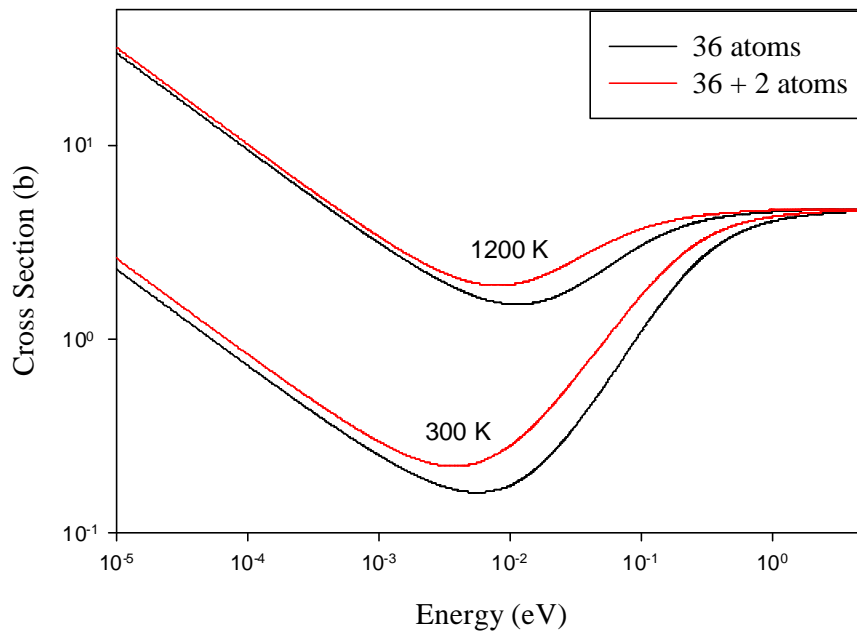# Phonon Frequency Distribution Single Interstitial

Thermal Scattering Cross Sections Single Interstitial

Phonon Frequency Distribution Di-interstitials

Thermal Scattering Cross Sections Di-Interstitials

Impact on VHTR Analysis and Design

☐ Variations in the thermal neutron scattering cross section affect the thermal neutron spectrum in the VHTR

☐ A spectrum harder/softer than predicted would imply different fuel needs to meet design goals and clearly affects the overall economic performance of the reactor

☐ The current safety conclusions may also be impacted. The analysis of a transient scenario may have to be altered to account better for moderator spectral effects